3-Deoxy-manno-oct-2-ulopyranosonic acid

10149-14-1 | DTXSID80143949

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.07 mol/L

Global applicability domain: Outside

Local applicability domain index: 4.18e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

Image not found
D-Gluconic acid
Measured: 1.61
Predicted: 1.83

Image not found
Sodium D-gluconate
Measured: 2.70
Predicted: 1.83

Image not found
Mucic acid
Measured: 2.29e-01
Predicted: 3.04e-01

Image not found
Mucic acid
Measured: 2.29e-01
Predicted: 3.04e-01

Image not found
D-Glucitol
Measured: 1.45
Predicted: 1.49

Image not found
D-Mannitol
Measured: 1.45
Predicted: 1.49

Image not found
D-Galactitol
Measured: 1.45
Predicted: 1.49